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Solid hydrogen doped with energetic impurities may form the basis for HEDM to be used in rocket propulsion. A key research priority was therefore the largescale computer simulation of impurity diffusion and recombination in HEDM in order to better understand the reasons for its stability, or instability, as the case may be. The recombination of these atomic impurities is an extremely exothermic reaction, and therefore thermodynamically favored. Theoretical developments within our research group allowed for the (otherwise impossible) quantum dynamical simulation of these systems which was necessary to properly treat the problem. Classical molecular dynamics simulations, while less computationally challenging, predict qualitatively incorrect properties for low temperature liquid and solid hydrogen because of the highly quantum nature of hydrogen matrix, and are therefore inadequate.

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AFOSR Final Report

Computer Simulations of Low Temperature High Energy Density Materials
(F49620-96-1-0129)

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Introduction: Low Temperature HEDM Simulations

Solid hydrogen doped with energetic impurities may form the basis for HEDM to be used in rocket propulsion. A key research priority was therefore the largescale computer simulation of impurity diffusion and recombination in HEDM in order to better understand the reasons for its stability, or instability, as the case may be. The recombination of these atomic impurities is an extremely exothermic reaction, and therefore thermodynamically favored. Theoretical developments within our research group allowed for the (otherwise impossible) quantum dynamical simulation of these systems which was necessary to properly treat the problem. Classical molecular dynamics simulations, while less computationally challenging, predict qualitatively incorrect properties for low temperature liquid and solid hydrogen because of the highly quantum nature of hydrogen matrix, and are therefore inadequate.

The immediate goal of the research project was to calculate directly from largescale computer simulation the relevant rates for the impurity recombination process. In low temperature hydrogen HEDM, quantum effects are enormous, so a highly specialized method is required for these demanding computer simulations.

This grant lasted only for one year at the University of Pennsylvania because the P.I. moved to the University of Utah.

Summary of Key Results:

The primary result was the largescale quantum calculation of the intrinsic lithium impurity recombination rate in para-hydrogen at 4K.

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